Argonne NATIONAL LABORATORY

ESP Kick-Off Workshop Introduction

Plan, legalities, introductions, overview

Presenter: Tim Williams (ALCF)

October 18, 2010

Legalities and Security

- **Workshop open only to registered participants**
  - Your name badge is your pass
- **IBM AECI agreements**
  - Agreement for Exchange of Confidential Information
  - Each individual's home institution must have signed
    - Base agreement
    - Blue Gene/Q Supplement
  - Confidentiality of Blue Gene/Q information
    - Unsure if information is confidential? Email earlyscience@alcf.anl.gov
- **Please treat Workshop materials, discussions as confidential**
  - Next-generation Blue Gene/Q hardware specifics
  - Software for Blue Gene/Q

AECI signed with 30 institutions

Who's Here?

- **77 participants from 23 institutions**
- **Representatives from Early Science Program projects**
  - 39 People, 16 institutions
- **7 IBM representatives**
- **12 ALCF Catalysts & Performance Engineers**
  - Applications/technical questions
- **Libraries, Tools, and Programming Models Project partipants**
  - Kalyan Kumaran (Kumar)
  - 26 People, 9 institutions
- **Robert Scott (ALCF User Services)**
  - Accounts, login, CRYPTOCards
- **Sue Gregurich (ALCF)**
  - Workshop logistics

Plan for Workshop

- **IBM talks on Blue Gene/Q**
  - Hardware
  - Software
  - Performance, simulator
  - Compilers
  - Messaging
- **GFDL preliminary performance results**
- **15-minute ESP project presentations**
  - Current code, methods, parallelism, dependencies
  - Needs for Blue Gene/Q
  - Plan for next 6 months
- **From ALCF/MCS**
  - Performance tools plans
  - Programming models
  - Mira acceptance-test applications
  - ALCF I/O plans
  - BG/Q Tools Project
- **Breakout Session (Tools project)**
  - Performance monitors update
- **Working Lunches**
  - Help with ALCF resources
  - Discuss ESP postdocs
  - Plan future workshops
- **RECEPTION TONIGHT**

Group Photo – Monday 3:30 Coffee Break

Early Science Program

- **ALCF Next-Generation IBM Blue Gene/Q machine *Mira***
  - Delivered 2012
  - Production 2013
- ***N* Months between acceptance and production: *Early Science Period***
  - 2 billion core-hours dedicated to ESP Projects
    - 12-15 projects ➔ large blocks computer time
    - Must burn time fast
      - 2 years to get ready
      - Mira has ~5X cores of present-day Blue Gene/P machine Intrepid
        - » 20X as fast (10 petaFLOPS)
      - Prepare applications to scale
        - » Node-level parallelism

ESP Projects

- **Call for proposals April 2010**
- **40 viable proposals submitted**
- **16 awards**
  - Target usage on Mira (50 – 150 million core hours)
  - Development time on Intrepid (4 – 15 million core hours over 2 years)
  - About 15 postdoctoral positions focusing on ESP projects
  - Collaboration with ALCF staff and IBM

Science Area Representation

	Awarded Projects	All 40 Proposals
Chemistry	2	4
Nuclear Structure	2	2
Biology	2	4
Materials	1	2
Astro/Cosmology	2	8
Climate	1	4
Fusion	1	2
Geophysics	1	1
Combustion	2	2
Plasma	0	2
Energy	1	1
Computer Science	0	2
CFD/Aero	1	5
Atomic Physics	0	1

Institutional Representation

	Awarded Projects	All 40 Proposals
National Labs	7	14
Universities	10	24
Industry	0	1

National Representation

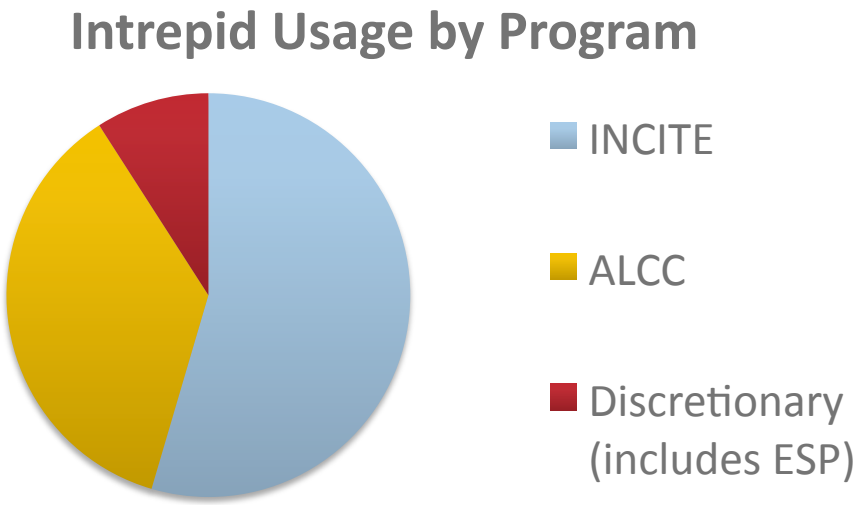
	Awarded Projects	All 40 Proposals
United States	15	37
Foreign	1	3

Algorithm/Method Representation

	Awarded Projects	All 40 Proposals
Structured Grids	8	25
Unstructured Grids	5	19
FFT	6	19
Dense Linear Algebra	3	9
Sparse Linear Algebra	4	12
Particles/N-Body	5	11
Monte Carlo	2	2

Develop on Present-Day ALCF Machines

- **ALCF's Blue Gene/P machine, *Intrepid***
  - 40K nodes, 160K cores
  - 3D torus primary interconnect
  - 2 GB per node
  - 8 PB online disk
- **ESP allocations for *development***
  - Prepare applications for Mira



INCITE: **N**ovel **C**omputational **I**mpact on **T**heory and **E**xperiment

ALCC: **A**SCR **L**eadership **C**omputing **C**hallenge

ASCR: DOE Office of **A**dvanced **S**cientific **C**omputing **R**esearch

END

ESP Proposal Solicitation and Review

- **Forthcoming Call for Proposals publicized**
  - SC09 talks at ANL booth by Messina and Riley
  - Flyer mailed to all ALCF users (about 500) on 18 December 2009
- **January 29, 2010 – Call for proposals issued**
  - ALCF website, INCITE website, ANL main website,
  - Email to over 800 people: INCITE and Discretionary ALCF users, 2009 INCITE proposal submitters, BlueGene Consortium, ad hoc list including SciDAC recipients
- **April 29, 2010 – Call for proposals closed**
- **Proposal Review**
  - Computational Readiness: 2-3 ALCF staff reviewers per proposal
  - Science Impact: 1-2 reviewers with science domain expertise (from ALCF, ANL, and larger scientific communities)
  - Ranking process resulting in recommendations
    1. Numerical scores from 2 review phases
    2. Group discussion by ALCF staff reviewers
    3. ALCF and CELS management discussion
- **PIs notified of results August 6, 2010**

Library and Tool Usage

NOT SHOWN: MPI, MPI-IO, OpenMP

	Recommended	All 40 Proposals
NetCDF	3	5
HDF	5	11
VisIt	2	6
ParaView	2	5
IDL	1	1
FFTW, FFTPACK5, P3DFFT, ESSL FFT	5	11
BLAS, ESSL BLAS	4	5
LAPACK	2	6
ScaLAPACK	1	3
MASS, MASSV, ESSL	1	3
parMETIS	1	1
PETSc	1	1
Python	1	4
Tau	0	1
Scalasca	0	1
Charm++	2	3
Chombo	1	1
GASNet	1	1

COLORS: BG/Q PORT
Kumar's tool effort
IBM
Other efforts